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Microscopic and thermodynamic properties of dense semiclassical partially ionized hydrogen plasma

T S Ramazanov, K N Dzhumagulova and M T Gabdullin

IETP, Al-Farabi Kazakh National University, 96a, Tole Bi St, Almaty, 050012, Kazakhstan

E-mail: ramazan@physics.kz

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Abstract

Microscopic and thermodynamic properties of dense semiclassical partially ionized hydrogen plasma were investigated on the basis of pseudopotential models. Radial distribution functions (RDF) of particles were obtained using a system of the Ornstein–Zernike integral equations. The corrections to internal energy and the equation of state were calculated using RDF.

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1. Introduction

In this work we consider the dense semiclassical partially ionized hydrogen plasma consisting of electrons, ions and atoms. Number density changes in the range of $n = n_e + n_i = 10^{20}$–10^{24} cm^{-3} and the temperature domain is 5×10^4–10^6 K.

It is convenient to describe the plasma state with dimensionless parameters which characterize the dimension of physical values such as numerical density. Coupling parameter Γ characterizes the potential energy of interaction in comparison with the thermal energy: $\Gamma = (Ze)^2/ak_BT$, where $= \sqrt[3]{3/4\pi n_e}$ is the average distance between particles. For weakly coupled plasma $\Gamma < 1$. The density parameter is the relation of average distance to the Bohr radius: $r_S = a/a_B$, where $a_B = \hbar^2/e^2m_e$ is the Bohr radius. The degree of degeneracy for the electrons is measured by the ratio of the thermal energy to the Fermi energy: $\Theta = k_BT/E_F = 2\,(4/9\pi)^{2/3}\,Z^{5/3}r_s/\,\Gamma$, where E_F is the Fermi energy for electrons. The condition $\Theta \geqslant 1$ corresponds to the state of weak and intermediate degeneracy.

2. Interaction models

Various approaches are used for the description of plasma properties with different parameters. In the calculation of thermodynamic functions of nonideal plasma, we have difficulties related to the interaction of particles. There are also especial difficulties in investigations of partially ionized plasma properties since it is necessary to know the interaction potentials. Such potentials should take into account the specific effects existing in the considered area of densities and temperatures. A pseudopotential model that takes into consideration the quantum-mechanical and screening effects was used for the description of interaction between charged particles [1]

$$\Phi(r) = \frac{Ze^2}{\sqrt{1-4\lambda^2/r_D^2}}\left(\frac{e^{-Ar}}{r} - \frac{e^{-Br}}{r}\right), \tag{1}$$

where $\lambda = \hbar/\sqrt{2\pi m k_B T}$ is the thermal de Broglie wavelength, $r_D = \sqrt{k_B T/4\pi n_e e^2}$ is the Debye radius, $A = \sqrt{\left(1-\sqrt{1-4\lambda 1^2/r_D^2}\right)/2\lambda^2}$, $B = \sqrt{\left(1+\sqrt{1-4\lambda^2/r_D^2}\right)/2\lambda^2}$.

The influence of atoms on the thermodynamic properties of a partially ionized plasma increases with decreasing free electron number density. The interaction between a charge and an atom in plasma is basically caused by effects of polarization and is of short range character. The screening version of the Buckingham potential was chosen as the potential of the charge–atom interaction in partially ionized nonideal plasma [2]:

$$\Phi_{ea}(r) = -\frac{e^2\alpha_D}{2\left(r^2+r_0^2\right)^2}\exp\left(-\frac{2r}{r_D}\right)\times\left(1+\frac{r}{r_D}\right)^2, \tag{2}$$

where α_D is the atom polarizability, r_0 is the cutoff radius of the atom. The value of the dipole polarizability for the hydrogen atom is $\alpha_D = 4.5a_B^3$, the cutoff radius of the atom is $r_0 = 1.4565a_B$ [3].

In the second case, we used the polarization potential of the charge–atom interaction [4]

$$\Psi_{es}(r) = -\frac{e^2\alpha}{2r^4\left(1-4\lambda^2/r_D^2\right)}\left(e^{-Br}(1+Br)(1-B^2\lambda^2) - e^{-Ar}(1+Ar)(1-A^2\lambda^2)\right)^2. \tag{3}$$

It is supposed that diffraction effects are also taken into account in considerations of atom–electron interactions.

3. Ionization equilibrium in hydrogen plasma

In the investigation of plasma composition, we used the nonlinear Saha equation with corrections to nonideality (lowering of ionization potentials) [5]

$$\frac{1-\alpha}{\alpha^2} = n\lambda^3\exp\left[\frac{I-\Delta I}{k_B T}\right], \tag{4}$$

where I, ΔI are the ionization potential and lowering of ionization potential for hydrogen, respectively. The lowering of ionization potential can be described in the following form:

$$\Delta I = -\sqrt{3}\Gamma^{\frac{3}{2}} - \frac{3}{2}\Gamma^2 - \frac{3\sqrt{3}}{2}\Gamma^{\frac{5}{2}} - \frac{\Gamma^3}{\pi r_s} + \frac{1}{\sqrt{1+3\Gamma}}(2.5\Gamma + 5.8\Gamma^2). \tag{5}$$

The ionization coefficient $\alpha = n_e/n$ characterizes the ratio of the number density of free electrons to the number density of electrons in plasma.

The Saha equation was solved to obtain the plasma ionization stages at different densities and temperatures. The ionization states of hydrogen plasma are presented in figure 1.

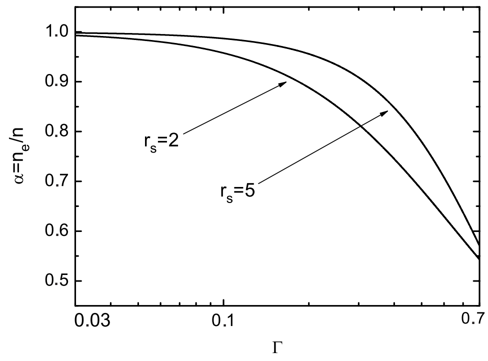

Figure 1. Ionization rate as a function of coupling parameter.

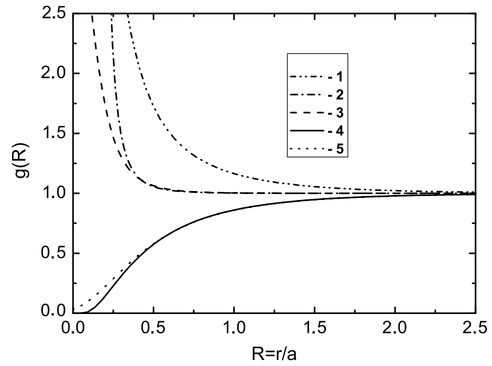

Figure 2. RDF between particles at $r_s = 5$ and $\Gamma = 0.3$ for different effective potentials: 1—electron–proton, formula (1); 2—electron–atom, (3), 3—electron–atom, formula (2), 4—proton–proton, (1), 5—electron–electron, (1).

4. Radial distribution functions of particles

Radial distribution functions of particles were obtained by solving a system of the Ornstein–Zernike integral equations. The Ornstein–Zernike equations connect the full and direct correlation functions with the interaction potential of particles:

$$h(\vec{r}) = c(\vec{r}) + n \int c(\vec{r} - \vec{r}')h(\vec{r}')\,\mathrm{d}\vec{r}', \tag{6}$$

where $h(\vec{r}) = g(\vec{r}) - 1$ is a full correlation function, $c(\vec{r})$ is a direct correlation function. Equation (6) is written in the following form in the hypernetted chain approximation of dense semiclassical hydrogen plasma consisting of electrons, ions and atoms:

$$h_{ab}(\vec{r}) = c_{ab}(\vec{r}) + \sum_{d=1}^{3} n_d \int c_{ad}(\vec{r} - \vec{r}')h_{db}(\vec{r}')\,\mathrm{d}\vec{r}'. \tag{7}$$

The Fourier transform and direct iterative methods were used for the calculation of the system of equations (7).

Calculated RDFs are presented in figure 2.

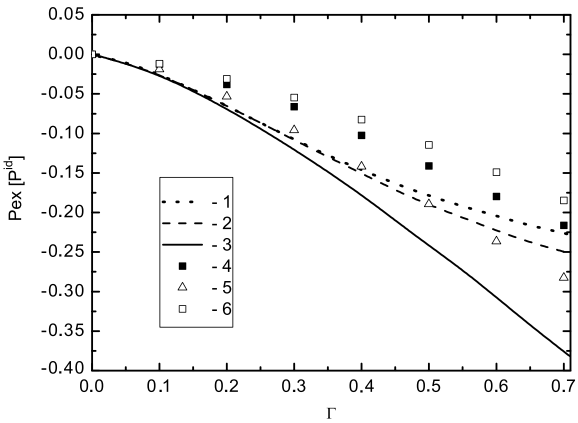

Figure 3. Excess pressure of hydrogen plasma at $r_s = 5$: 1—formula (2); 2—formula (3); 3—fully ionized plasma; 4—[6] with $A_0 = \frac{\pi}{2}$; 5—[6] with $A_0 = 0$; 6—[7].

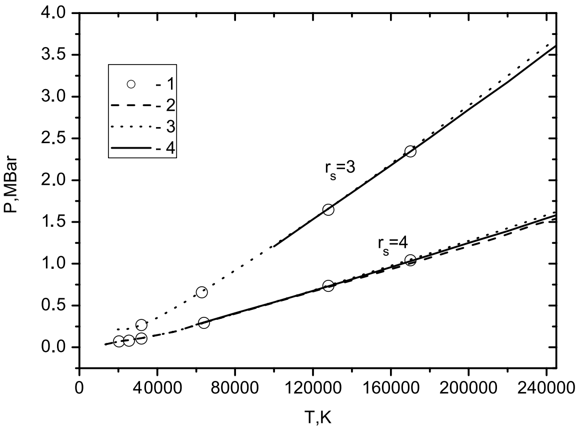

Figure 4. Comparison of pressure versus temperature for deuterium: 1—PIMC [8]; 2—SC [9]; 3—ACTEX [10]; 4—present work.

5. Thermodynamic properties of dense semiclassical partially ionized hydrogen plasma

Interaction corrections to the thermodynamic functions of a nonideal system have been derived from the radial distribution functions of particles in this system. Hence, the excess pressure and the excess internal energy may be written as:

$$P_{ex} = -\frac{2}{3}\pi \sum_{a=i,e,n} n_a \sum_{b=i,e,n} n_b \int_0^\infty \frac{\partial \Phi_{a,b}(r)}{\partial R} g_{a,b}(r) r^3 \, \mathrm{d}r, \tag{8}$$

$$E_{ex} = \pi \sum_{a=i,e,n} n_a \sum_{b=i,e,n} n_b \int_0^\infty \Phi_{a,b}(r) g_{a,b}(r) r^2 \, \mathrm{d}r, \tag{9}$$

where the summation is performed over all sorts of particles (electrons, ions and atoms). These expressions were calculated by numerical methods.

The obtained excess pressure and excess internal energy are presented in figures 3 and 5 as functions of coupling Γ and density r_s parameters. At a fixed density parameter r_s, the

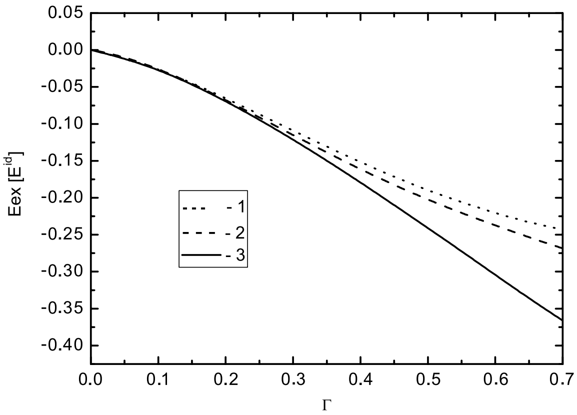

Figure 5. Excess internal energy of hydrogen plasma at $r_s = 5$ for different effective potentials: 1—formula (2); 2—formula (3); 3—fully ionized plasma.

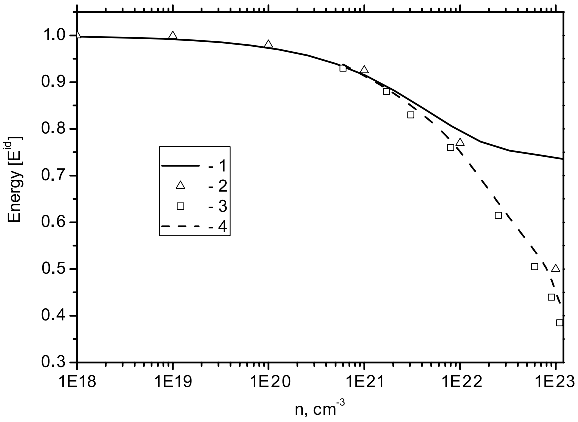

Figure 6. Energy of dense hydrogen plasma at $T = 125\,000$ K: 1—present work; 2—[11]; 3—[12]; 4—[13].

influence of the neutral component in the system becomes evident with increasing coupling parameter. It suggests a decrease of excess pressure and excess internal energy for partially ionized plasma in comparison with a fully ionized one. Figure 4 presents a curve of pressure versus temperature in comparison with results obtained by other authors for several values of r_s. One can see that these four approaches agree well. Figure 6 gives results for the total energy of hydrogen at $T = 125\,000$ K. The agreement up to number densities of the order 10^{22} cm^{-3} is quite good. However, starting with number densities 10^{22} cm^{-3} our curve lies above the curves of other authors. This depends on the degree of ionization α. At a fixed number density, the values α in this work are smaller than the data of the works [11–13].

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